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Exhaled breath analysis using full-scan SIFT-MS data: development of chemometric approaches and clinical potential

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Abstract: The ballistic rise of analytical technologies has opened a large playground for all type of untargeted “omics” screening. In that trend, there is a rising interest for the characterization of the human volatilome. Indeed, the characterization and the understanding of the volatile organic compounds (VOCs) production in different ex vivo matrices could open the route for improved diagnosis approaches and more individualized treatments.

For large-scale screening, direct introduction instruments, such as selected ion flow tube mass spectrometry (SIFT-MS) offer the capacity to perform both targeted and untargeted analyses within a few minutes. SIFT-MS can generate compositional patterns from direct sample introduction at the same time than other routine medical actions. However, the use of SIFT-MS for untargeted screening requires the acquisition of full-scan mass spectra for every precursors of interest. To investigate this type of data, multiple factors such as the different chemistries of each precursor and structure of the data set, have to be taken into account to extract useful information.

In this pilot study, we investigated the potential of full-scan SIFT-MS for breath-based asthma phenotyping. The first step was the development of specific chemometric tools for the optimization and the exploitation of the SIFT-MS data. Targeted and untargeted approaches have been applied and compared to evaluate their potential to translate into the clinic.

Pierre-Hugues Stefanuto is lead scientist and lecturer at Liège University in Belgium. His main research interest is the development of analytical solutions based on chromatography and mass spectrometry technology. He is interested in the development of statistical models for method optimization and data handling. He is working on the development of multimodal solutions for untargeted screening of small molecules.

Driving Research Goal: Development of multi-omics screening to tackle biomedical challenges at the molecular level